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APPLICATION OF THE MCCABE-THIELE METHOD BY MEANS OF MATHEMATICAL MODELING IN EXCEL TO DETERMINE THE THEORETICAL STAGES OF A BINARY DISTILLATION

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Abstract: This study focuses on the simulation of a binary distillation process of ethanol and water using a model developed in Excel, with the aim of obtaining ethanol with a purity of 90%. Distillation is widely recognized as one of the most common separation methods in the chemical industry, and the case of ethanol-water is especially relevant due to its industrial applications in the production of biofuels and in the pharmaceutical industry. For the simulation, a feed with a molar flow of 100 kmol/h was used, with an equimolar composition of ethanol and water. Using the McCabe-Thiele method, an equilibrium diagram was developed that represents the relationship between the vapor and liquid compositions in each phase of the process. From this analysis, the theoretical stages required and the optimal location of the feed tray were calculated to maximize the efficiency of the distillation column. The model allowed obtaining a distillate with a molar flow of 75 kmol/h and a residue of 25 kmol/h. The results indicated that 10.6 theoretical stages are required to reach the desired purity of 90% ethanol in the distillate. The simulation also highlighted the importance of the early stages in the separation process, where the greatest difference in composition between the vapor and liquid phases is observed. This study demonstrates the feasibility of using Excel as an accessible tool for simulating distillation processes, especially in educational and preliminary research contexts. It also highlights the effectiveness of the McCabe-Thiele method in the design and analysis of distillation columns, offering results that align with theoretical principles and industrial practice.
Keywords: Ethanol, binary distillation, McCabe-Thiele, equilibrium diagram.

INTRODUCTION

Distillation is a thermal separation process based on differences in the volatilities of components in a liquid mixture. This method has been widely used in the chemical, petrochemical and food industries due to its ability to separate and purify compounds with high efficiency (GHOUFI; ARTZNER; MALFREYT, 2016). In particular, the binary distillation of ethanol and water is a highly relevant process in the production of ethanol, which is widely used as a biofuel, in the pharmaceutical industry and in the production of alcoholic beverages (YAN; EDGAR; BALDEA, 2019).

The design and optimization of distillation columns are fundamental tasks in the field of chemical engineering, since these processes require considerable consumption of energy and material resources. The McCabe-Thiele method, developed in the 1920s, is a graphical tool that has been fundamental in the teaching and practice of distillation column design (BARDERAS, 2010). This method makes it possible, through a simplified approach, to calculate the number of theoretical stages required to achieve the desired separation between two components in a mixture. (ZAPATA BENABITHE et al., 2020).

Although there are numerous commercial software designed for the simulation of distillation processes, such as Aspen HYSYS and ChemCAD, the use of Excel for this purpose offers an accessible and versatile alternative. Excel not only facilitates the implementation of mathematical models and the visualization of data, but also allows engineers and students to perform preliminary simulations without the need for specialized software (HU et al., 2020).

This study aims to apply an Excel model to simulate the binary distillation process of ethanol and water, in order to produce ethanol with a purity of 90%. Through this simulation, we seek to demonstrate the effectiveness of the McCabe-Thiele method and highlight the usefulness of Excel as an accessible and effective modeling tool in the context of chemical engineering (POTHOCZKI; PUSZTAI; BAKÓ, 2018).

METHODOLOGY

SYSTEM DESCRIPTION

The system studied consists of a binary distillation column that separates a mixture of ethanol and water. This process is carried out at atmospheric pressure, and the column feed is set at a molar flow of 100 kmol/h, with an equimolar composition of ethanol and water (OCON; TOJO, 1980). The design of the system is based on the essential principles of distillation, using the differences in the volatilities of the components to achieve the desired separation. (KONG; MARAVELIAS, 2019).

GENERAL AND SPECIFIC SUBJECT BALANCE

The overall material balance applied to the distillation process is expressed as:

$$F = D + R \qquad (1)$$

F, *D, R* is the molar flow of feed, distillate and residue respectively.

The material balance for the most volatile component, in this case ethanol, is formulated as follows:

$$Fx_F = Dx_D + Rx_R \qquad (2)$$

x_F, x_D and x_R are the molar fractions of ethanol in the feed, distillate and residue, respectively [2].

MINIMUM REFLUX AND OPERATING REFLUX

Minimum reflux is the ratio of the amount of liquid recirculated to the column to the amount of vapor condensed, required to achieve the desired separation with an infinite number of theoretical plates. This parameter is essential to define the operating limits of the distillation column (A. UDUGAMA et al., 2018). Operating reflux, on the other hand, refers to the actual reflux ratio used in the column, lying between the extremes of total reflux (minimum number of plates) and minimum reflux (infinite number of plates) (YANG et al., 2019). The equation used to calculate the operating reflux is:

$$R_{op} = nR_{min} \qquad (3)$$

where n is an adjustment factor that depends on the specific operating conditions of the column (ASPRION, 2020).

LINES OF OPERATION

In the McCabe-Thiele method, two main operating lines are considered: the line of enrichment (LOE) and the line of depletion (LOA). The enrichment line corresponds to the section of the column located between the feed point and the upper tray, while the depletion line is located between the feed point and the lower tray (ALVES et al., 2020).

The equation of the operating line for the enrichment section is expressed as:

$$y_{n+1} = \frac{L_n}{V_{n+1}} x_n + \frac{D_{x_D}}{V_{n+1}} \qquad (4)$$

Where:

- y_{n+1} is the molar fraction of ethanol in the rising vapor,
- x_n is the molar fraction of ethanol in the liquid that goes down,
- L_n and V_{n+1} are the molar flows of liquid and vapor at the respective stages.

The component balance or operating line in the enrichment section is formulated as:

$$y_{n+1} = \frac{R}{R+1} x_n + \frac{X_D}{R+1} \qquad (5)$$

This equation is essential to define the behavior of the mixture within the column and to determine the number of stages required for separation (KUMAR; GHOSH; PAL, 2019).

DETERMINATION OF THE THEORETICAL STAGES

The theoretical stages are determined using the McCabe-Thiele Graphic method, which involves plotting steps between the operating line and the equilibrium curve. These steps represent the stages of contact between the liquid and vapor phases within the column. (SHANG et al., 2019).

LOCATION OF THE FEEDING DISH

The feed tray location is determined in the McCabe-Thiele diagram by the intersection of the enrichment operation line with the feed line (SEEDAT; KAUCHALI; PATEL, 2021). This cut-off point defines the optimal position for introducing the feed into the column, which maximizes the process efficiency (LIU et al., 2021).

THERMAL CONDITION OF THE FEED

The thermal condition of the feed, represented by the parameter q, is critical in determining the slope of the feed line in the McCabe-Thiele diagram (KIRSCHNER et al., 2021). The parameter q is defined as the molar fraction of saturated liquid formed per mole of feed material, and its value varies depending on the feed condition, as shown in the following Table.

Feeding conditions	Thermal condition measurement "q"
Subcooled liquid	$q > 1$
Saturated liquid	$q = 1$
Partially vaporized	$1 > q > 0$
Saturated steam	$q = 0$
Superheated steam	$q < 0$

Table 1: Conditions of feeding

LIQUID-VAPOR EQUILIBRIUM

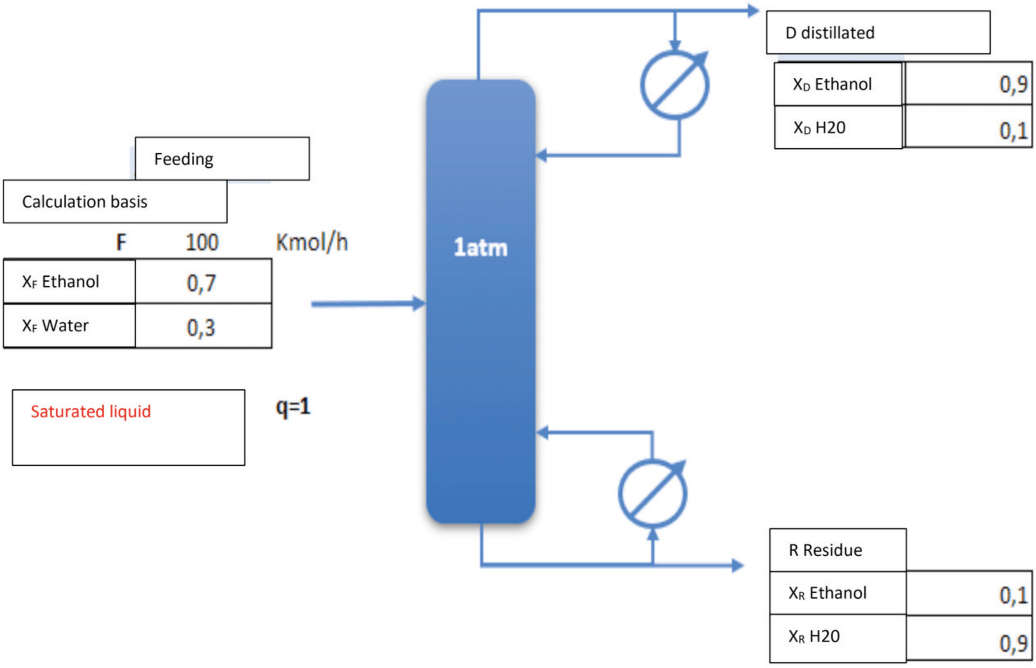
Liquid-vapor equilibrium is essential for the design and analysis of distillation processes. In the case of the binary ethanol-water system, equilibrium data at 1 atm pressure are used to plot the equilibrium curve on the McCabe-Thiele diagram (LEJEUNE; RABILLER-BAUDRY; RENOUARD, 2018), allowing the determination of the number of theoretical stages and the optimal position of the feed plate (MARCILLA, 1998).

EXCEL IMPLEMENTATION AND MODEL VALIDATION

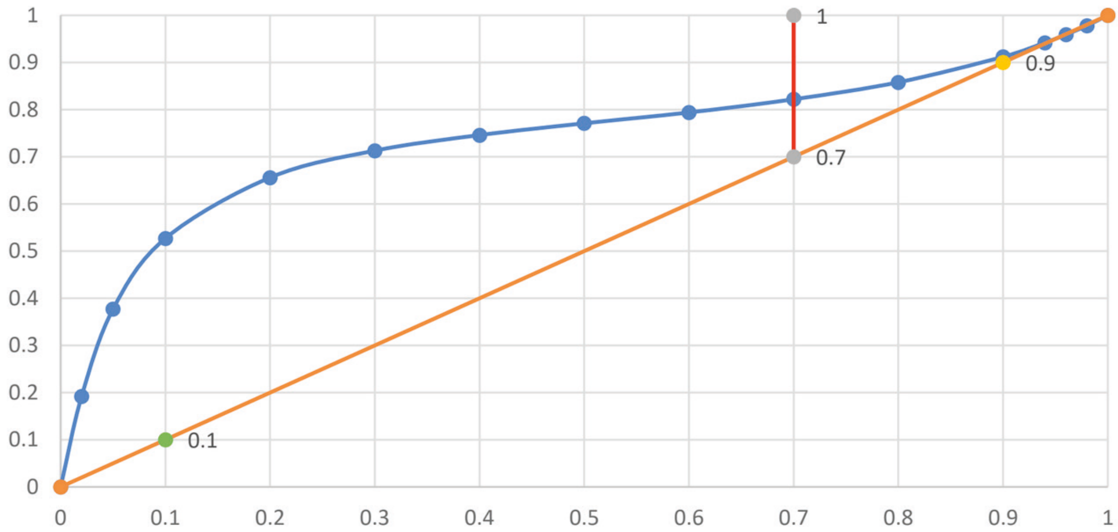
The mathematical model and the equations presented were implemented in Excel, using iteration and graphics functions to simulate the distillation process (FOUST; WENZEL; CLUMP, 1984). The simulation allowed obtaining the theoretical number of stages, the minimum reflux, and the optimal location of the feed plate. The validation of the model was carried out by comparing the results obtained with experimental data and simulations in specialized software, demonstrating the accuracy and usefulness of the approach used (KONG; MARAVELIAS, 2019).

T °C	95.5	89	86.7	85.3	82.7	81.5	79.8	79.3	78.41	78.15
x	0.019	0.072	0.096	0.124	0.23	0.32	0.50	0.57	0.74	0.894
y	0.17	0.389	0.427	0.47	0.54	0.58	0.65	0.68	0.78	0.894

Table 2: Ethanol-water equilibrium system at 1 atm



Graphic 1: The flow chart



Graphic 2: Ethanol-water equilibrium system at 1 atm

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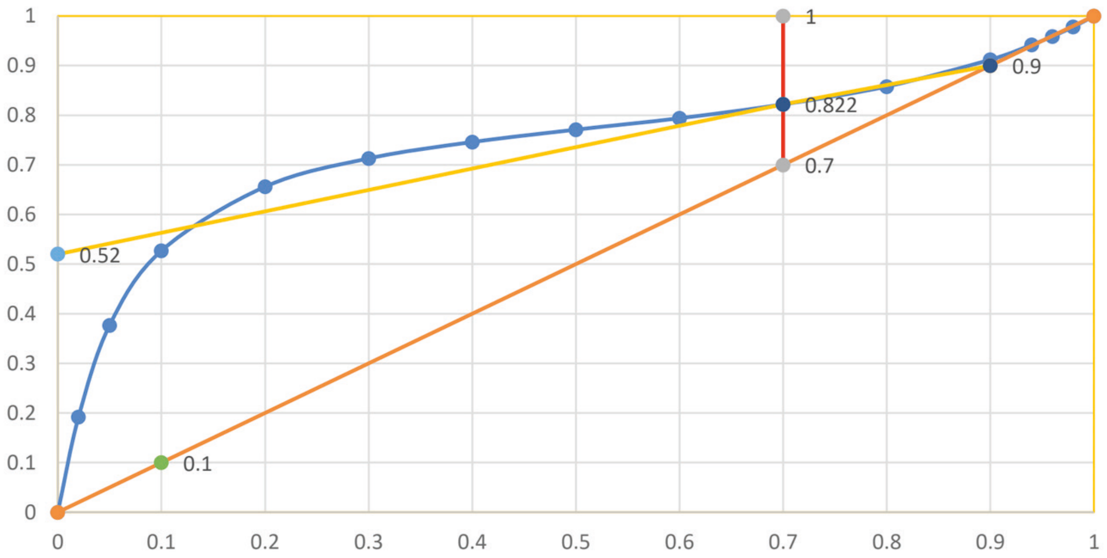


Graphic 3: Ethanol-water equilibrium diagram at 1 atm

RESULTS AND DISCUSSION

The Excel tool will be used to perform a distillation of a mixture of ethanol and water, starting with a composition of 70% ethanol and 30% water at a pressure of 1 atm. The feed mixture, in a saturated liquid state (q=1), will enter the column, and the objective is to obtain a distillate with a 90% ethanol fraction. The McCabe-Thiele method will be used to calculate the number of theoretical stages required and the feed plate. (VEINTIMILLA, 2022).

Variables	Values
$x_{F\ \text{ethanol}}$	0.7
$x_{F\ \text{water}}$	0.3
P (atm)	1
Saturated liquid (q)	1
$x_{D\ \text{ethanol}}$	0.9

Table 3: Data presented

Figure 1 presents the flowsheet for binary distillation with the conditions specified in Table 3. Since the feed was not specified in terms of flow, a feed rate of 100 kmol/h will be assumed for the calculations (CARRAVETTA et al., 2022).

The results obtained from the Excel simulation showed that, for a feed molar flow of 100 kmol/h and using the McCabe-Thiele method, it was possible to obtain a distillate with an ethanol purity of 90%, corresponding to a distillate flow of 75 kmol/h and a residue of 25 kmol/h.

In Illustration 3, the trace of the line from xD that crosses a point that touches the equilibrium curve and q is shown, finally intercepting the y axis, giving b= 0.52 (VEINTIMILLA, 2022)

The calculation of the theoretical number of stages is carried out through the operating line of the enrichment section, which is related to the vapor-liquid composition. In this case, the enrichment line equation is used. Then, by replacing the data, the value of the minimum reflux (Rmin) is obtained, which in this case is b=0.52, which is obtained on the y-axis of the drawn line (VEINTIMILLA, 2022).

Enrichment line equation

$$y = \frac{R}{R+1}x + \frac{x_D}{R+1}$$

The slope formula

$$y = m\,x + b$$

We substituted and the equation is:

$$b = \frac{x_D}{R_{min}+1}$$

$$0.52 = \frac{0.9}{Rmin + 1}$$

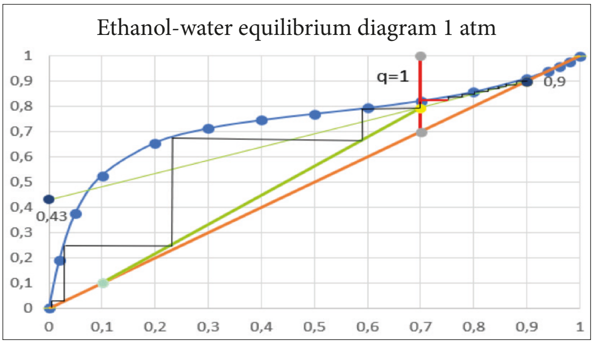
$$Rmin = 0,7308$$

Calculate the reflux of Rop operation and rectification line.

$$Rop = n\,Rmin$$
$$Rop = 1.5\ (0.7308)$$
$$Rop = 1.0962$$

$$\frac{X_D}{Rop + 1}$$
$$\frac{0.9}{1.0962 + 1} = \mathbf{0.43}$$

We draw the new rectification line on the graph, and: 0.43. In illustration 4, the results of the number of theoretical stages and feed plate can be observed by the graphical method.



Graphic 4: Number of theoretical stages

The calculated number of theoretical stages was 10.6, with a feed tray located at the eighth stage. These results are consistent with the theoretical principles of distillation and the McCabe-Thiele method, confirming that the Excel modeling can reproduce the expected behavior of the ethanol-water system under the stated conditions.

The analysis of the equilibrium diagram allowed to identify the liquid-vapor equilibrium compositions at each stage, observing that most of the separation occurs in the early stages, where the composition difference between vapor and liquid is most significant. This behavior is typical in binary distillation systems and underlines the importance of proper column design to optimize separation.

CONCLUSION

The study demonstrated that it is possible to use Excel to simulate a binary ethanol-water distillation process with a high degree of accuracy, using the McCabe-Thiele method. The results obtained are not only consistent with theory, but also underline the accessibility and utility of Excel as an alternative tool for modelling distillation processes in educational or preliminary research settings.

Excel's ability to perform iterative calculations and visualise results makes it a viable option for those without access to specialised simulation software, providing a solid foundation for the design and analysis of separation processes in the chemical industry.

REFERENCES

ALVES, J. L. F. et al. Ethanol enrichment from an aqueous stream using an innovative multi-tube falling film distillation column equipped with a biphasic thermosiphon. **Process Safety and Environmental Protection**, v. 139, p. 69–75, jul. 2020.

ASPRION, N. Modeling, Simulation, and Optimization 4.0 for a Distillation Column. **Chemie Ingenieur Technik**, v. 92, n. 7, p. 879–889, 29 jul. 2020.

A. UDUGAMA, I. et al. Side draw control design for a high purity multi-component distillation column. **ISA Transactions**, v. 76, p. 167–177, maio 2018.

BARDERAS, V. A. **Destilación Por El Metodo de Mc Cabe - Thiele.** [s.l: s.n.].

CARRAVETTA, V. et al. An atomistic explanation of the ethanol–water azeotrope. **Physical Chemistry Chemical Physics**, v. 24, n. 42, p. 26037–26045, 2022.

FOUST, A.; WENZEL, L.; CLUMP, C. **Principios de Operaciones Unitarias**. México : CECSA, 1984.

GHOUFI, A.; ARTZNER, F.; MALFREYT, P. Physical Properties and Hydrogen-Bonding Network of Water–Ethanol Mixtures from Molecular Dynamics Simulations. **The Journal of Physical Chemistry B**, v. 120, n. 4, p. 793–802, 4 fev. 2016.

HU, Y. et al. Design and optimization of the efficient extractive distillation process for separating the binary azeotropic mixture methanol-acetone based on the quantum chemistry and conceptual design. **Separation and Purification Technology**, v. 242, p. 116829, jul. 2020.

KIRSCHNER, J. et al. The molecular structure of the surface of water–ethanol mixtures. **Physical Chemistry Chemical Physics**, v. 23, n. 19, p. 11568–11578, 2021.

KONG, L.; MARAVELIAS, C. T. From graphical to model-based distillation column design: A McCabe-Thiele-inspired mathematical programming approach. **AIChE Journal**, v. 65, n. 11, 7 nov. 2019.

KUMAR, R.; GHOSH, A. K.; PAL, P. Fermentative ethanol production from Madhuca indica flowers using immobilized yeast cells coupled with solar driven direct contact membrane distillation with commercial hydrophobic membranes. **Energy Conversion and Management**, v. 181, p. 593–607, fev. 2019.

LEJEUNE, A.; RABILLER-BAUDRY, M.; RENOUARD, T. Design of membrane cascades according to the method of McCabe-Thiele: An organic solvent nanofiltration case study for olefin hydroformylation in toluene. **Separation and Purification Technology**, v. 195, p. 339–357, abr. 2018.

LIU, S. et al. [EMIM][DCA] as an entrainer for the extractive distillation of methanol-ethanol-water system. **Green Energy & Environment**, v. 6, n. 3, p. 363–370, jun. 2021.

MARCILLA, A. **Introducción a Las Operaciones de Separación. Cálculo Por Etapas de Equilibrio.** Espagrafic ed. España: Publicaciones Universidad de Alicante, 1998.

OCON, P.; TOJO, J. **Problemas de Ingeniería Química**. [s.l.] Aguilar, 1980.

POTHOCZKI, S.; PUSZTAI, L.; BAKÓ, I. Temperature dependent dynamics in water-ethanol liquid mixtures. **Journal of Molecular Liquids**, v. 271, p. 571–579, dez. 2018.

SEEDAT, N.; KAUCHALI, S.; PATEL, B. A graphical method for the preliminary design of ternary simple distillation columns at finite reflux. **South African Journal of Chemical Engineering**, v. 37, p. 99–109, jul. 2021.

SHANG, X. et al. Process analysis of extractive distillation for the separation of ethanol–water using deep eutectic solvent as entrainer. **Chemical Engineering Research and Design**, v. 148, p. 298–311, ago. 2019.

VEINTIMILLA, K. **Determinación de las etapas teóricas y plato de alimentación mediante el método de mc cabe-thiele en la destilación binaria.** Machala : ``Universidad Técnica de Machala``, 2022.

YANG, A. et al. Energy-efficient extractive pressure-swing distillation for separating binary minimum azeotropic mixture dimethyl carbonate and ethanol. **Separation and Purification Technology**, v. 229, p. 115817, dez. 2019.

YAN, L.; EDGAR, T. F.; BALDEA, M. Dynamic Process Intensification of Binary Distillation via Periodic Operation. **Industrial & Engineering Chemistry Research**, v. 58, n. 15, p. 5830–5837, 17 abr. 2019.

ZAPATA BENABITHE, Z. et al. Caso de estudio de la destilación etanol-agua en operación continua y discontinua y su simulación con ecuaciones cúbicas de estado y modelos de actividad. **TecnoLógicas**, v. 23, n. 49, p. 223–249, 15 set. 2020.